

OMSO2 README File

Date: 12/20/2006

Authors: N.A. Krotkov, K. Yang, S.A. Carn, and A. Krueger

PGE version 1.0.0 ECS collection 2

Overview

This document describes the SO₂ product (OMSO2) retrieved from global mode measurements of the Ozone Monitoring Instrument (OMI) on the EOS AURA satellite in a sun-synchronous ascending polar orbit (1:45pm local equator crossing time). The product file, called a granule, contains estimates of the total SO₂ (vertical column in Dobson Units, where 1DU=2.69 X 10¹⁶ molecules/cm²), adjustments to OMTO3 total ozone and Lambertian equivalent reflectivity, and ancillary information produced by the OMSO2 algorithm. Each granule (~20Mb) covers the sunlit portion of the orbit with an approximately 2600 km wide swath containing 60 pixels per viewing line. During normal operations, 14 or 15 granules are produced daily, providing fully contiguous coverage of the globe.

The three reported total SO₂ values correspond to three *a-priori* vertical profiles for the SO₂ vertical distribution used in the retrieval algorithm. The three vertical profiles were selected to represent typical SO₂ vertical distributions for three SO₂ source regimes: SO₂ in the Planetary Boundary Layer (PBL, below 2 km) from anthropogenic sources, SO₂ distributed between 5 and 10 km emitted by passive volcanic degassing in the free troposphere, and SO₂ distributed between 15 and 20 km representing injection from explosive volcanic eruptions. The user is advised to select one SO₂ value most consistent with the expected SO₂ vertical distribution for their specific application.

In the OMSO2 data there is cloud screening. The screened regions contain fill values. The screening criteria are different for PBL and 5km data (see Data Quality Assessment). One should see no fill values due to cloud screening in the 15KM data.

The accuracy and precision of the SO₂ data vary significantly with the SO₂ loading and vertical profile, observational geometry, slant column ozone and in the presence of sub-pixel clouds and aerosols. Preliminary error estimates are discussed below (see Data Quality Assessment). However, due to the combination of a smaller footprint and measurements at wavelengths that are highly sensitive to SO₂ absorption, the minimum SO₂ mass detectable by OMI is two orders of magnitude lower than the detection threshold of the NASA Total Ozone Mapping Spectrometer (Krueger et al 1995; <http://toms.umbc.edu>).

Documentation and examples of detected SO₂ emissions are available from our main web site (<http://so2.umbc.edu/omi>). Details about software versions and known issues are available in the OMSO2ReleaseDetails file (<http://so2.umbc.edu/omi/Documentation/OMSO2ReleaseDetails.html>).

Algorithm Description

In the OMSO2 product, all PBL data are processed with the Band Residual Difference (BRD) method (Krotkov, et al 2006), while all 5 km and 15 km data are processed with the Linear Fit (LF) algorithm. The algorithms use different subsets of calibrated residuals produced by the NASA operational ozone algorithm (OMTO3: <http://toms.gsfc.nasa.gov/omi/OMTO3Readme.html>). This set contains residuals centered at the Earth Probe (EP) TOMS wavelengths, four residuals at extrema of the SO₂ absorption cross-section from 310.8-314.4 nm, and two non-absorbing wavelengths at 345 and 370 nm. Both OMSO2 algorithms use the temperature-dependent SO₂ cross-sections data (Bogumil et al 2000), residual correction for background regions, and different parameterizations of the Air Mass Factors (AMF).

When the atmospheric SO₂ loading is low (<10 DU), the BRD algorithm is suitable for SO₂ retrieval. The BRD algorithm uses differential residuals at 3 SO₂ sensitive OMI UV2 wavelength pairs, and the pair average is used to produce all PBL data. A constant AMF of 0.36 is used to estimate total SO₂ (vertical column). This value represents idealized cloud and aerosol free sky conditions, slant column ozone (SCO; given by total ozone*(secSZA+secVZA)) of ~1000DU, 5% surface albedo, a typical summer PBL SO₂ vertical profile and 1 DU SO₂ load. The greater is the difference between the actual and the assumed idealized observational conditions, the larger is the error in PBL SO₂ (see Data Quality Assessment). **Therefore, off-line AMF corrections should always be considered before using OMI SO₂ data for estimating SO₂ emissions.** These include mandatory corrections for SO₂ amount and vertical profile, total ozone, viewing geometry, surface albedo, aerosols and clouds. Useful examples of the recommended AMF corrections are given in OMSO2AMFcorrections file (<http://so2.umbc.edu/omi/Documentation/OMSO2AMFcorrections.html>). We will also provide off-line AMF corrections upon user request (see contact information).

For strong volcanic degassing and eruptions, SO₂ loading can be very large and the BRD algorithm may fail. The LF algorithm has been developed to optimally select residuals from the set of available OMTO3 bands to retrieve SO₂ under these conditions (<http://so2.umbc.edu/omi/Documentation/LinearFitAlgorithmDescription.html>). The LF algorithm minimizes a subset of the residuals by simultaneously adjusting total SO₂, total column ozone, reflectivity at 331nm, and polynomial coefficients (linear and quadratic) to account for the wavelength dependent effect of surface albedo and aerosol on the effective reflectivity.

Data Quality Assessment

Instrument calibration, forward model, and OMTO3 retrieval errors in the residual wavelengths are compensated by subtracting the median residual in SO₂- free background pixels from the observed residuals. The median is computed for each viewing angle from a sliding group of 350 pixels along the orbit track. SO₂-contaminated and bad pixels are excluded from the median calculation if the OMTO3

error flag is equal or greater than 5. In addition, BRD pairs consistent with real SO₂ and with slant column SO₂ greater than 2 DU are excluded.

We provide separate Quality Flags (QF) for each of the products that are based on SO₂ consistency criteria between the individual wavelength pairs. The OMSO₂ pixel quality flag is an automatic assessment of the SO₂ values for the corresponding pixel by the OMSO₂ retrieval algorithm. It is used primarily as an indicator of the validity of the volcanic SO₂ values. A user of OMSO₂ data is advised to examine the first bit of the quality flag. If this bit is equal to zero, the retrieved SO₂ value is likely to be good. But if it is equal to 1, this indicates that during the retrieval, the algorithm has determined that the pixel does not exhibit characteristics that are consistent with the presence of SO₂. Also the quality flag includes other information, such the geometrical and geophysical conditions, that are relevant to the quality of SO₂ retrieval. For detailed information about the SO₂ quality flag, please consult the OMSO₂.fs file specification (<http://so2.umbc.edu/omi/Documentation/OMSO2.fs.html>)

The pixel quality flags in OMSO₂ are not yet fully functional. Preliminary analysis of the QF values has shown that they work best for large volcanic events, but miss many real PBL and low level degassing emissions. **Users are advised to ignore QF and use independent verification of PBL SO₂ emissions.**

Below are data quality assessments for each SO₂ product after applying moving median residual correction and ignoring QF. For all data, the noise level in the South Atlantic radiation Anomaly is increased.

PBL data

The slant column (SC) PBL SO₂ data produced with the BRD algorithm feature a practically zero global mean bias (typically within 0.1DU) and a global background noise level of about 0.6 DU (1 standard deviation) based on a preliminary survey of the data. Using a constant AMF of 0.36, this translates into a ~0.2 DU bias and 1.7 DU noise in global total SO₂ values, while regional noise levels vary significantly. With this sensitivity, daily detection of plumes from strong volcanic degassing and anthropogenic sources of SO₂ (such as smelters and coal burning power plants) may be possible. However, any individual SO₂ value for a specific pixel may be questionable due to the large standard deviation of PBL SO₂ values. Therefore, at least weekly or longer time period maps of PBL SO₂ are of greater value, but artifacts are still possible.

We provide diagnostic information in the OMSO₂ product, intended to help distinguish real PBL SO₂ signals from artifacts. For example, SO₂ can be computed independently from each of the BRD pairs and the difference between pair solutions would indicate errors in the calibration or retrieval assumptions, or unusual meteorological situations. Comparison between SO₂ data produced with BRD (PBL data) and LF (5km and 15km data) algorithms is also recommended when possible to confirm the presence of SO₂. In unclear cases PGE developers will provide off-line verifications using Spectral Fit (SF) algorithm upon user request (see contact information).

Assuming that detected SO₂ is real, additional errors arise if observational conditions differ from those assumed in the AMF parameterization. For example, AMF of 0.36 is underestimated by 20% for SCO=700 DU (small ozone, solar zenith and nadir angles), but overestimated by ~30% for SCO=1500 DU. For even larger SCO values (high ozone and/or high solar and viewing angles, mostly at high latitudes), AMF becomes very small, so no good PBL SO₂ retrieval is expected. Therefore, fill values are reported for pixels with SCO>1500DU.

In addition, aerosols and subpixel clouds can affect the AMF in different ways depending on their location. The assumption is that clouds always screen PBL SO₂, but no AMF correction is attempted to account for this invisible SO₂. This cloud related AMF error becomes larger with increasing sub-pixel cloudiness, so that fill values are used if OMTO3 cloud fraction is larger than ~20%, which corresponds to LER ~30%. **Even for low reflectivities, off-line AMF corrections should always be considered before using OMI SO₂ data for estimating SO₂ emissions.** Useful examples of the recommended AMF corrections are given in OMSO2AMFcorrections file (<http://so2.umbc.edu/omi/Documentation/OMSO2AMFcorrections.html>). We will also provide off-line AMF corrections upon user request.

Volcanic 5 km data

The 5 km retrievals are intended to represent typical volcanic outgassing from tall volcanoes and emissions from effusive eruptions. We recommend that the 5 km retrievals be used for volcanic degassing cases at all altitudes because the PBL retrievals are restricted to clear sky situations and contain large artifacts when sub-footprint clouds are present. The cloud-related fill values are possible in 5km data when the assumed cloud top (from OMTO3 climatology) is higher than 10 km. In such cases the cloud blocks most of the 5KM SO₂. As a result, SO₂ weighting function becomes close to zero and no LF retrieval is done and the fill value is stored in the output. Examples are given in OMSO2ReleaseDetails file (<http://so2.umbc.edu/omi/Documentation/OMSO2ReleaseDetails.html>).

In general, SO₂ releases at altitudes less than 5 km will be underestimated due to errors in the AMF, but these could be corrected in an off-line processing if degassing altitude is known. Biases in the 5 km retrievals due to latitude and viewing angle are removed to the 0.1 DU level by the median residual background offset corrections. The standard deviation of 5 km retrievals in background areas is about 0.3 DU at low and mid-latitudes. Both the bias and standard deviations increase for solar zenith angles greater than 80°. Cross track striping has been found near the northern terminator in some orbits. The known artifacts in the OMTO3 residuals are due to 1) errors in ozone retrievals over tropical cloud edges (positive errors ~ 1DU) 2) ozone profile errors in anomalous meteorological situations, e.g. cut-off low pressure systems at mid-latitudes (negative SO₂ errors of ~ -1 DU), and 3) from the possible errors in the cloud top pressure used in the retrieval of total ozone in OMTO3 algorithm.

Volcanic 15 km data

The 15 km retrievals are intended for use with explosive volcanic eruptions where the cloud is placed in the upper troposphere or stratosphere. At these altitudes the AMF is weakly dependent on altitude, so that differences in actual cloud height from 15 km produce only small errors.

The biases with latitude and viewing angle are generally less than 0.1 DU. The noise level in background data is about 0.2DU. . Both the bias and standard deviation increase near the northern terminator, similar to but reduced from the 5 km results. Artifacts due to ozone profile errors and cloud edges are reduced from the 5 km data by about 30%. One should see no fill values due to cloud screening in the 15KM data.

The LF algorithm still has large error when it comes to high SO₂ loading cases. The LF algorithm as implemented in the v1.0.0 OMSO₂ is expected to provide good retrieval when SO₂ loading is less than ~30 DU. When SO₂ loadings are higher than ~50DU the LF algorithm underestimates the true SO₂ amount, the higher the loading the larger the underestimation.

Product Description

The OMSO₂ product is written as HDF-EOS5 swath file. For a list of tools that read HDF-EOS5 data files, please visit this link:

<http://disc.gsfc.nasa.gov/Aura/tools.shtml>

A file, also called a granule, contains SO₂ and associated information retrieved from each OMI pixel from the sun-lit portion of an Aura orbit. The data are ordered in time sequence. The information provided on these files includes: latitude, longitude, solar zenith angle, OMTO3 reflectivity (LER) and independent estimates of the SO₂ vertical columns, as well as a number of ancillary parameters that provide information to assess data quality. Three values of SO₂ VC are provided corresponding to three assumed vertical profiles. Independent information is needed to decide which value is most applicable. For a complete list of the parameters, please read the OMSO₂ file specification: (<http://so2.umbc.edu/omi/Documentation/OMSO2.fs.html>)

Questions related to the OMSO₂ dataset should be directed to the GES DAAC, (<mailto:help@daac.gsfc.nasa.gov>). Users may consult the OMI Quality Assessment Team (omiqa@ssaihq.com) for the most recent information on OMI data quality. For questions and comments related to the OMSO₂ algorithm and data quality please contact Nickolay Krotkov (krotkov@mhatter.gsfc.nasa.gov), who has the overall responsibility for this product, with copies to Kai Yang (Kai.Yang.1@gsfc.nasa.gov), Arlin J. Krueger (akrueger@umbc.edu), and Simon Carn (scarn@umbc.edu).

References

Bogumil, K., J. Orphal, T. Homann, S. Voigt, P. Spietz, O.C. Fleischmann, A. Vogel, M. Hartmann, H. Kromminga, H. Bovensmann, J. Frerick, J.P. Burrows, Measurements of molecular absorption spectra with the SCIAMACHY pre-flight model: instrument characterization and reference data for atmospheric remote-sensing in the 230-2380nm region, *Journal of Photochemistry and Photobiology, A:Chemistry*, 157 , 167-184, 2003.

Krotkov, N.A., S.A. Carn, A.J. Krueger, P.K. Bhartia, and K. Yang (2005). Band residual difference algorithm for retrieval of SO₂ from the Aura Ozone Monitoring Instrument (OMI). *IEEE Trans.Geosci. Remote Sensing, AURA special issue*, 44(5), 1259-1266, doi:10.1109/TGRS.2005.861932, 2006

Krueger, A.J., L.S. Walter, P.K. Bhartia, C.C. Schnetzler, N.A. Krotkov, I. Sprod, and G.J.S. Bluth(1995). Volcanic sulfur dioxide measurements from the total ozone mapping spectrometer instruments. *J. Geophys. Res.*, 100(D7), 14057-14076, 10.1029/95JD01222.